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DRUG DISCOVERY LABS LOOK TO THE DIGITAL FUTURE

AS INFORMATIC TOOLS EVOLVE, researchers can look forward to a future where integrated systems combine knowledge and execution during experiments.

With more than 25 years in the scientific software space, David Gosalvez has dedicated his career to developing digital tools that accelerate research in the life sciences. As executive director of science and technology at Revvity Signals Software, he leads the teams behind the company's next-generation software and prototypes innovative new products. The scientific challenges behind drug discovery are more formidable than ever, so what does the future look like for the technologies designed to help researchers go further, faster? Gosalvez shares his insights on opportunities for digitalization in the pharmaceutical and biotech industries.

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When did informatic tools become a fundamental component of drug discovery work?
It's been very gradual. We were developing electronic notebooks as early as 2003, which were rudimentary compared to what we have today. Labs recognized that it was better to track things electronically than manually. The next wave, since around 2010, was about analytics. And in the last decade or so, the focus has shifted to getting value out of the data, and more sophisticated tools to understand and make decisions based on that data.

What do you see as some of the biggest pain points for scientists?
As an industry, we developed this piecemeal, application-centric ecosystem. As a scientist, that's not appealing. It certainly doesn't meet the expectations of the young, digital-native scientist. You might have to use six different systems before noon just to do your job, and spend half your day assembling data, reformatting it, and reorganizing it so it'll make sense in the next context.

Over the last five years or so, we've started really building to the scientist's workflow. For example, if your job is to design and build new antibodies, what do you need, from soup to nuts? And that goes from how you organize your thoughts, to how you generate your experimental parameters, to how you capture your data. It's never a single system, but it's vital to reduce the number of systems and integrate those systems with workflows.

What are the next steps in this direction?
Can that more comprehensive platform be properly integrated with the other systems that are in the environment? That's the forefront: the ways in which you integrate these systems. And by systems, I mean software platforms that may differ on what they deliver, as well as lab instruments and equipment. It's about making your workforce more efficient, because you can begin to automate things that otherwise take up a lot of research time.

Where do you think rapidly evolving AI capabilities are going to fit in the drug discovery toolbox?
Obviously, the whole AI thing is popular right now, and some of it will stick and some of it will not. One thing I think is here to stay is less experimentation and more prediction. As an industry, we have the capabilities and desire to do more *in silico*. Experimentation is expensive, and so even simple things like reducing the number of permutations that you do in an experiment represent a huge efficiency gain. In 10 years we will be doing less hands-on experimentation, and more modelling, simulation, prediction, and *in silico* design. AI is going to play a major role in getting us there.

Are there areas where you think the potential benefits of AI are being overstated?
It doesn't matter what technology you pick; it isn't going to be the panacea. AI is going to be an important tool, but it's not going to replace the scientist. It doesn't replace creative thought, the primary human contribution. Anybody who's pitching the idea that we're going to have a pharmaceutical company that's just a bunch of computers sitting in the corner and running Chat GPT — that's an overstatement of the reality. So, I am wary of the 'too good to be true', which there's a lot of out there.

Are there emerging digital trends that you think are underappreciated?
The revolution to me is in novel therapeutic approaches. We've spent a lot of time doing small-molecule pharmaceutical therapies, and for a number of years we've moved into larger, more complex biologics. That's already a pretty mainstream thing. The frontier is the evolution of other therapeutic approaches, which are neither large nor small molecules. Things like cell therapies, where you're literally taking cells out of a patient, modifying them, and giving them back. Or gene therapies, or the vaccines we just developed for COVID. The tools for those new modalities aren't there yet — they haven't caught up. So how rapidly can the industry produce technique-appropriate tooling? That's an area of focus for us now, really understanding what these researchers do, what they need, and what we can provide to them quickly. That will have an impact on the next generation of therapies.

How do you see the nature of the scientist's job changing as the digital toolbox evolves?

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▲ As digital tools evolve, drug discovery labs will do less hands-on experimentation and more modelling, simulation and in silico design, says Gosalvez.

I think the fundamentals are the same. What changes is the drudgery. People don't have a clue how much low-value, repetitive, boring, error-prone operations these very well-educated people are doing day-to-day. If you look five, ten years from now, I see a scientist being more of a scientist and less of a grunt. And when you talk about the new generation — as scientists, they don't have the patience or the desire to be grunts; they expect technology to solve those things.

What excites you about the future of the digital laboratory?
I think machines will know more about what the scientist wants to accomplish. Part of what we do at Revvity is build really sophisticated instruments. But that's only part of it. You've got to know how to run the instrument, how to set it up for the problem you're trying to solve. I see a possibility where you can walk up to your instrument and say, "I'm trying to accomplish this task." And that knowledge can be processed by the machine, which says, "I understand what you're trying to do. I am able to set up the parameters and the experiment." It's the melding of our knowledge with the intelligent machine, which right now requires too much human intervention. A lot of this can be done with AI — often, it's simpler AI things, or narrow AI, that we're not doing right now as opposed to this kind of magical general AI world where the machine learns how to do the science and the scientists stay home. The vision is to build integrated systems that combine the human knowledge with the machine's execution. ■

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